



# Sharp bounds on the zeroth-order general Randić index of unicyclic graphs with given diameter<sup>☆</sup>

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## ABSTRACT

Let  $G$  be a simple connected graph and  $\alpha$  be a given real number. The zeroth-order general Randić index  ${}^0R_\alpha(G)$  is defined as  $\sum_{v \in V(G)} [d_G(v)]^\alpha$ , where  $d_G(v)$  denotes the degree of the vertex  $v$  of  $G$ . In this work, we give, for any  $\alpha (\neq 0, 1)$ , some sharp bounds on the zeroth-order general Randić index  ${}^0R_\alpha$  of all unicyclic graphs with  $n$  vertices and diameter  $d$ .

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## 1. Introduction

Given a simple connected graph  $G = (V(G), E(G))$ , where  $V(G)$  and  $E(G)$  denote the sets of vertices and edges of  $G$ , respectively, the Randić index of  $G$  is defined as [1]

$$R(G) = \sum_{(u,v) \in E(G)} [d_G(u)d_G(v)]^{-\frac{1}{2}},$$

where  $d_G(u)$  denotes the degree of the vertex  $u$  of  $G$ . Randić himself demonstrated [1] that this index is well correlated with a variety of physico-chemical properties of various classes of organic compounds. The Randić index and some of its variants have received intensive attention and have been generalized in many ways. In particular, the zeroth-order general Randić index is defined in [2] as

$${}^0R_\alpha(G) = \sum_{v \in V(G)} [d_G(v)]^\alpha,$$

where  $\alpha$  is a real number. Some nice results can be found in the literature [2–13].

In this work, we investigate extremal values of general  ${}^0R_\alpha$  for simple connected unicyclic graphs of  $n$  vertices and diameter  $d$  and give some sharp bounds for this class of graphs. Since  ${}^0R_0(G) = |V(G)|$  and  ${}^0R_1(G) = 2|E(G)|$ , we only consider  $\alpha \neq 0, 1$ .

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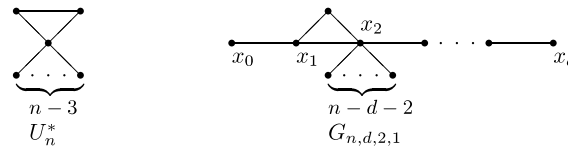


Fig. 1. The graphs in Introduction.

Now we introduce some definitions and notation. For undefined graph-theoretical terminology and notation the reader may refer to [14]. A *unicyclic* graph is a connected simple graph of  $n$  vertices and  $n$  edges. For two vertices  $u, v \in V(G)$  ( $u \neq v$ ), the *distance* between  $u$  and  $v$ , denoted by  $d_G(u, v)$ , is the number of edges in a shortest path joining  $u$  and  $v$  in  $G$ . The *diameter* of a graph  $G$ , denoted by  $\text{diam}(G)$ , is the maximum distance between any two vertices of  $G$ . A *pendent vertex* of a graph is a vertex with degree 1. Let  $C_n$  and  $P_n$  denote the cycle and path of  $n$  vertices, respectively. An edge is said to be *subdivided* when it is deleted and replaced by a path of length 2 connecting its ends, the internal vertex of this path being a new vertex. A *subdivision* of a graph  $G$  is a graph that can be obtained from  $G$  by a sequence of edge subdivisions. Let  $\mathcal{U}_{n,d}$  denote the set of all unicyclic graphs with order  $n$  and diameter  $d$ , where  $1 \leq d \leq n-2$ . Let  $U_n^*$  (shown in Fig. 1) denote the graph obtained from star  $S_n$  by adding a new edge between its two pendent vertices. Then  $\mathcal{U}_{n,1} = \{C_3\}$  (if  $n = 3$ ) or  $\emptyset$  (if  $n \geq 4$ ) and  $\mathcal{U}_{n,2} = \{U_4^*, C_4\}$  (if  $n = 4$ ) or  $\{U_5^*, C_5\}$  (if  $n = 5$ ) or  $\{U_n^*\}$  (if  $n \geq 6$ ). Denote by  $D(G) = (d_1, d_2, \dots, d_n)$  the degree sequence of the graph  $G$ , where  $d_i$  stands for the degree of the  $i$ th vertex of  $G$  and  $d_1 \geq d_2 \geq \dots \geq d_n$ . Let  $\mathcal{D}_n$  denote the set of sequences  $D = (d_1, d_2, \dots, d_n)$  of positive integers with  $d_1 \geq d_2 \geq \dots \geq d_n$  and  $\sum_{i=1}^n d_i = 2n$ . The *zeroth-order general Randić index* of a sequence  $D = (d_1, d_2, \dots, d_n)$  of positive integers is defined as

$${}^0R_\alpha(D) = \sum_{i=1}^n d_i^\alpha,$$

where  $\alpha$  is a real number. Note that  ${}^0R_\alpha(G) = {}^0R_\alpha(D(G))$  for any graph  $G$ .

Let  $D_1(n, d) = (n-d+1, 3, \overbrace{2, \dots, 2}^{d-2}, \overbrace{1, \dots, 1}^{n-d})$  and  $f_1(n, d, \alpha) = {}^0R_\alpha(D_1(n, d))$ .  
Let

$$D_2(n, d) = \begin{cases} D(C_n) = (\overbrace{2, \dots, 2}^n) & \text{if } d = \lfloor \frac{n}{2} \rfloor, \\ (3, \overbrace{2, \dots, 2}^{n-2}, 1) & \text{if } \lfloor \frac{n}{2} \rfloor < d \leq n-2, \end{cases}$$

and  $f_2(n, d, \alpha) = {}^0R_\alpha(D_2(n, d))$ , where  $3 \leq \lfloor \frac{n}{2} \rfloor \leq d \leq n-2$ .

Let  $P_d = x_0x_1 \dots x_d$  be a path of length  $d$ . Let  $G_{n,d,i,j}$  denote the graph obtained from  $P_d$  by attaching  $n-d-1$  pendent vertices to  $x_i$  and joining one of the new pendent vertices to  $x_j$ . For example,  $G_{n,d,2,1}$  is shown in Fig. 1. Let  $\mathcal{G}_{n,d} = \{G_{n,d,i,j} | 2 \leq i \leq d-1 \text{ and } 1 \leq j = i-1 \text{ or } i-2\}$ .

## 2. Lemmas

In this section, we give some lemmas that will be used in the proof of our result.

**Lemma 2.1** ([8]). If  $x-2 \geq y \geq 1$ , then

$$\begin{cases} (x-1)^\alpha + (y+1)^\alpha < x^\alpha + y^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ (x-1)^\alpha + (y+1)^\alpha > x^\alpha + y^\alpha & \text{if } 0 < \alpha < 1. \end{cases}$$

**Lemma 2.2** ([8]). If  $x \geq y \geq 2$ , then

$$\begin{cases} (x+1)^\alpha + (y-1)^\alpha > x^\alpha + y^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ (x+1)^\alpha + (y-1)^\alpha < x^\alpha + y^\alpha & \text{if } 0 < \alpha < 1. \end{cases}$$

**Lemma 2.3.** If  $D = (d_1, d_2, \dots, d_n) \in \mathcal{D}_n$  and there are two integers  $d_i, d_j$  such that  $d_i - 2 \geq d_j \geq 1$ , then there exists another sequence of integers  $D' \in \mathcal{D}_n$  satisfying

$$\begin{cases} {}^0R_\alpha(D) > {}^0R_\alpha(D') & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\ {}^0R_\alpha(D) < {}^0R_\alpha(D') & \text{for } 0 < \alpha < 1. \end{cases}$$

**Proof.** Let  $d'_i = d_i - 1$ ,  $d'_j = d_j + 1$  and  $d'_k = d_k$  for each  $k \in \{1, 2, \dots, n\} \setminus \{i, j\}$ . Rearrange  $d'_1, d'_2, \dots, d'_n$  as  $d'_{i_1} \geq d'_{i_2} \geq \dots \geq d'_{i_n}$ . It is not difficult to see that  $D' = (d'_{i_1}, d'_{i_2}, \dots, d'_{i_n}) \in \mathcal{D}_n$  and, by Lemma 2.1,

$${}^0R_\alpha(D) - {}^0R_\alpha(D') = d_i^\alpha + d_j^\alpha - (d_i - 1)^\alpha - (d_j + 1)^\alpha \begin{cases} > 0 & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\ < 0 & \text{for } 0 < \alpha < 1. \end{cases}$$

Then the proof of this lemma is complete.  $\square$

**Lemma 2.4.** If  $D = (d_1, d_2, \dots, d_n) \in \mathcal{D}_n$  and there are two integers  $d_i, d_j$  such that  $d_i \geq d_j \geq 2$ , then there exists another sequence of integers  $D' \in \mathcal{D}_n$  satisfying

$$\begin{cases} {}^0R_\alpha(D) < {}^0R_\alpha(D') & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\ {}^0R_\alpha(D) > {}^0R_\alpha(D') & \text{for } 0 < \alpha < 1. \end{cases}$$

**Proof.** Let  $d'_i = d_i + 1$ ,  $d'_j = d_j - 1$  and  $d'_k = d_k$  for each  $k \in \{1, 2, \dots, n\} \setminus \{i, j\}$ . Rearrange  $d'_1, d'_2, \dots, d'_n$  as  $d'_{i_1} \geq d'_{i_2} \geq \dots \geq d'_{i_n}$ . It is not difficult to see that  $D' = (d'_{i_1}, d'_{i_2}, \dots, d'_{i_n}) \in \mathcal{D}_n$  and, by Lemma 2.2,

$${}^0R_\alpha(D) - {}^0R_\alpha(D') = d_i^\alpha + d_j^\alpha - (d_i + 1)^\alpha - (d_j - 1)^\alpha \begin{cases} < 0 & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\ > 0 & \text{for } 0 < \alpha < 1. \end{cases}$$

Then the proof of this lemma is complete.  $\square$

The proof of the following lemma is not difficult and thus is omitted here (for a reference, see the Appendix).

**Lemma 2.5.** Let  $G \in \mathcal{U}_{n,d}$ , where  $3 \leq d \leq n - 2$ . Then  $D(G) = D_1(n, d)$  if and only if  $G \in \mathcal{G}_{n,d}$ .

### 3. Results

**Theorem 3.1.** Let  $G \in \mathcal{U}_{n,d}$ , where  $3 \leq d \leq n - 2$ . Then

$$\begin{cases} {}^0R_\alpha(G) \leq f_1(n, d, \alpha) & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\ {}^0R_\alpha(G) \geq f_1(n, d, \alpha) & \text{for } 0 < \alpha < 1. \end{cases}$$

Furthermore, the equalities hold if and only if  $G \in \mathcal{G}_{n,d}$ .

**Proof.** We only show Theorem 3.1 for the case of  $\alpha < 0$  or  $\alpha > 1$ , while the proof of Theorem 3.1 for  $0 < \alpha < 1$  is similar and thus omitted.

Assume  $\alpha < 0$  or  $\alpha > 1$  in the following.

Note that if  $G \in \mathcal{G}_{n,d}$ , then, by Lemma 2.5,  $D(G) = D_1(n, d)$  and  ${}^0R_\alpha(G) = f_1(n, d, \alpha)$ .

Assume  $G \in \mathcal{U}_{n,d}$  with  $D(G) = (d_1, d_2, \dots, d_{n-z}, \overbrace{1, 1, \dots, 1}^z)$ , where  $d_{n-z} \geq 2$ .

**Claim A.**  $0 \leq z \leq n - d$ .

In fact, let  $P = x_0x_1 \dots x_d$  and  $C$  be the shortest path of length  $d$  and the cycle in  $G$ , respectively; then  $d_G(x_i) \geq 2$  for all  $i = 1, 2, \dots, d - 1$  and there exists at least one vertex in  $V(C) \setminus V(P)$ . Thus there are at least  $d$  vertices of degree greater than 1. Then  $z \leq n - d$ . So Claim A is true.

Let  $D^* = (n + 2 - d, \overbrace{2, \dots, 2}^{d-1}, \overbrace{1, \dots, 1}^{n-d})$ . Then  $D^* \in \mathcal{D}_n$  and, by the proof of Lemma 2.4,  ${}^0R_\alpha(G) \leq {}^0R_\alpha(D^*)$ . In order for the equality to hold, we must have  $D(G) = D^*$ .

**Claim B.**  $D(G) = D^*$  if and only if  $G$  is isomorphic to a subdivision of  $U_{n+3-d}^*$ , denoted by  $G_1(n)$ , obtained from  $U_{n+3-d}^*$  by  $d - 3$  successive edge subdivisions.

Obviously, if  $G \cong G_1(n)$ , then  $D(G) = D^*$ . Conversely, assume  $D(G) = D^*$ . Let  $v \in V(G)$  be the vertex of maximum degree  $n + 2 - d$ . Then  $v$  is on the unique cycle of  $G$  (otherwise, there must be another vertex of degree more than 2). Thus  $G$  is isomorphic to some  $G_1(n)$ . So Claim B is true.

It is easy to see that  $\text{diam}(G_1(n)) \leq d - 1$ . Thus  $G_1(n) \notin \mathcal{U}_{n,d}$ . From the proof of Lemma 2.4, for each  $D(G)$ , where  $G \in \mathcal{U}_{n,d}$ , there is a sequence of integer sequences  $D'_1, D'_2, \dots, D'_s$  in  $\mathcal{D}_n$  such that  $D'_1 = D(G)$ ,  $D'_s = D^*$  and  $D'_{k+1}$ , where  $k = 1, 2, \dots, s - 1$ , is obtained from  $D'_k$  by an operation similar to that from  $D$  to  $D'$  in the proof of Lemma 2.4.

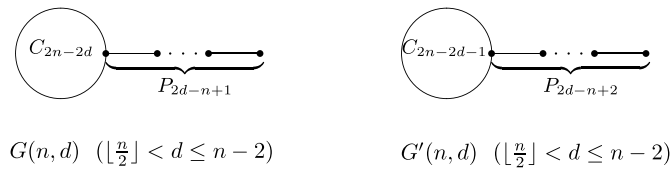


Fig. 2. The graphs in Theorem 3.2.

Then  ${}^0R_\alpha(D'_1) < {}^0R_\alpha(D'_2) < \dots < {}^0R_\alpha(D'_s)$ . For all  $G \in \mathcal{U}_{n,d}$ , either  $D'_{s-1} = (n+1-d, \overbrace{2, \dots, 2}^d, \overbrace{1, \dots, 1}^{n-d-1})$  or  $D'_{s-1} = (n+1-d, 3, \overbrace{2, \dots, 2}^{d-2}, \overbrace{1, \dots, 1}^{n-d}) = D_1(n, d)$ . By Lemma 2.1,

$${}^0R_\alpha((n+1-d, \overbrace{2, \dots, 2}^d, \overbrace{1, \dots, 1}^{n-d-1})) - {}^0R_\alpha(D_1(n, d)) = 2 \cdot 2^\alpha - 3^\alpha - 1^\alpha < 0.$$

Then  ${}^0R_\alpha((n+1-d, \overbrace{2, \dots, 2}^d, \overbrace{1, \dots, 1}^{n-d-1})) < {}^0R_\alpha(D_1(n, d))$ .

Therefore  ${}^0R_\alpha(G) \leq {}^0R_\alpha(D_1(n, d)) = f_1(n, d, \alpha)$  for all  $G \in \mathcal{U}_{n,d}$ . In order to have  ${}^0R_\alpha(G) = f_1(n, d, \alpha)$ , we must have  $D(G) = D_1(n, d)$ . By Lemma 2.5,  $G \in \mathcal{G}_{n,d}$ .

So Theorem 3.1 for the case of  $\alpha < 0$  or  $\alpha > 1$  is true.  $\square$

**Theorem 3.2.** Let  $G \in \mathcal{U}_{n,d}$ , where  $3 \leq \lfloor \frac{n}{2} \rfloor \leq d \leq n-2$ . Then

$$\begin{cases} {}^0R_\alpha(G) \geq f_2(n, d, \alpha) & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\ {}^0R_\alpha(G) \leq f_2(n, d, \alpha) & \text{for } 0 < \alpha < 1. \end{cases}$$

Furthermore, the equalities hold if and only if  $G \cong C_n$  for  $d = \lfloor \frac{n}{2} \rfloor$  or  $G \cong G_3(n, d)$  or  $G'_3(n, d)$  (shown in Fig. 2) for  $3 \leq \lfloor \frac{n}{2} \rfloor < d \leq n-2$ .

**Proof.** We only show Theorem 3.2 for the case of  $\alpha < 0$  or  $\alpha > 1$ , while the proof of Theorem 3.2 for  $0 < \alpha < 1$  is similar and thus omitted.

Assume  $\alpha < 0$  or  $\alpha > 1$  in the following.

Firstly, it is easy to check that if  $G \cong C_n$  or  $G(n, d)$  or  $G'(n, d)$ , then  $G \in \mathcal{U}_{n,d}$  and  $D(G) = D_2(n, d)$ . Thus  ${}^0R_\alpha(G) = f_2(n, d, \alpha)$ .

Let  $G \in \mathcal{U}_{n,d}$ . Then, by Lemma 2.3,  ${}^0R_\alpha(G) \geq {}^0R_\alpha(D_2(n, \lfloor \frac{n}{2} \rfloor))$ , where  $D_2(n, \lfloor \frac{n}{2} \rfloor) = (\overbrace{2, \dots, 2}^n)$ . In order for the equality to hold, we must have  $D(G) = D_2(n, \lfloor \frac{n}{2} \rfloor)$ . It is not difficult to see that  $D(G) = D_2(n, \lfloor \frac{n}{2} \rfloor)$  if and only if  $G \cong C_n$ .

Note that  $\text{diam}(C_n) = \lfloor \frac{n}{2} \rfloor$ . If  $3 \leq \lfloor \frac{n}{2} \rfloor < d \leq n-2$ , then  $C_n \notin \mathcal{U}_{n,d}$ . From the proof of Lemma 2.3, for each  $D(G)$ , where  $G \in \mathcal{U}_{n,d}$ , there is a sequence of integer sequences  $D'_1, D'_2, \dots, D'_s$  in  $\mathcal{D}_n$  such that  $D'_1 = D(G)$ ,  $D'_s = D_2(n, \lfloor \frac{n}{2} \rfloor)$  and  $D'_{k+1}$ , where  $k = 1, 2, \dots, s-1$ , is obtained from  $D'_k$  by an operation similar to that going from  $D$  to  $D'$  in the proof of Lemma 2.3.

Then  ${}^0R_\alpha(D'_1) > {}^0R_\alpha(D'_2) > \dots > {}^0R_\alpha(D'_s)$  and for all  $G \in \mathcal{U}_{n,d}$ ,  $D'_{s-1} = (3, \overbrace{2, \dots, 2}^{n-2}, 1) = D_2(n, d)$ .

Therefore  ${}^0R_\alpha(G) \leq {}^0R_\alpha(D_2(n, d)) = f_2(n, d, \alpha)$  for all  $G \in \mathcal{U}_{n,d}$ . In order to have  ${}^0R_\alpha(G) = f_2(n, d, \alpha)$ , we must have  $D(G) = D_2(n, d)$  and thus  $G \cong G(n, d)$  or  $G'(n, d)$  where  $3 \leq \lfloor \frac{n}{2} \rfloor < d \leq n-2$ .

So Theorem 3.2 for the case of  $\alpha < 0$  or  $\alpha > 1$  is true.  $\square$

#### 4. Remark

In this work, we give partial sharp bounds for the zeroth-order general Randić index for all unicyclic graphs with given diameter. For  $3 \leq d < \lfloor \frac{n}{2} \rfloor$ , the upper (resp. lower) bounds of  ${}^0R_\alpha(G)$  for  $0 < \alpha < 1$  (resp.  $\alpha < 0$  or  $\alpha > 1$ ) for  $G \in \mathcal{U}_{n,d}$  are still not established.

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## Appendix

**Proof of Lemma 2.5.** Firstly, if  $G \in \mathcal{G}_{n,d}$ , then it is easy to see that  $G \in \mathcal{U}_{n,d}$  and  $D(G) = D_1(n, d)$ .

Secondly, let  $G \in \mathcal{U}_{n,d}$  with  $D(G) = D_1(n, d)$ , where  $3 \leq d \leq n-2$ . Let  $P = x_0x_1 \dots x_d$  be a shortest path of length  $d$  in  $G$ . Then  $d_G(x_i) \geq 2$  for all  $i = 1, \dots, d-1$ . Since  $D(G) = D_1(n, d)$ , there are just  $d$  vertices of degree greater than 1 in  $G$ . If one of the vertices with maximum degree is not in  $\{x_1, x_2, \dots, x_{d-1}\}$ , then there exists  $i \in \{1, 2, \dots, d-1\}$  such that  $d_G(x_i) = 3$  and  $d_G(x_j) = 2$  for all  $j \in \{1, 2, \dots, d-1\} \setminus \{i\}$ , since  $G$  has only two vertices of degree  $\geq 3$ . Evidently,  $d_G(x_k) \neq n-d+1$  for  $k = 0, d$  (otherwise, the diameter of  $G$  is greater than  $d$ ). Then  $V(C) \cap V(P) = \emptyset$ , where  $C$  is the unique cycle of  $G$ . Thus there are at least  $d+2$  vertices with degree  $\geq 2$ . This is a contradiction to  $D(G) = D_1(G)$ . Consequently, there exists  $i' \in \{1, 2, \dots, d-1\}$  such that  $d_G(x_{i'}) = n-d+1$ . If  $d_G(x_{i'}) = n-d+1 = 3$ , then, by the previous reasoning, there exists  $j' \in \{1, 2, \dots, d-1\} \setminus \{i'\}$  with  $d_G(x_{j'}) = 3$ , since there are two vertices of maximum degree 3 in  $G$ . Then  $|j' - i'| \leq 2$  and there is a vertex  $u$  of  $G$  such that  $ux_{i'}, ux_{j'} \in E(G)$ , since  $G \in \mathcal{U}_{n,d}$  and  $D(G) = D_1(n, d)$ . Without loss of generality, assume  $j' < i'$ . Then  $G \cong G_{n,n-2,i',j'}$ , where  $1 \leq j' = i' - 1$  or  $i' - 2$ . Thus  $G \in \mathcal{G}_{n,n-2}$ . Otherwise, if  $d_G(x_{i'}) = n-d+1 \geq 4$ , then we claim that the unique vertex  $v$  of degree 3 is in  $\{x_1, x_2, \dots, x_{d-1}\} \setminus \{x_{i'}\}$ . In fact, if  $v \in V(G) \setminus V(P)$ , then there are at least  $d+1$  vertices with degree  $\geq 2$ , a contradiction to  $D(G) = D_1(n, d)$ . So  $v \in V(P)$ . If  $v \in \{x_0, x_d\}$ , then  $G$  has more than  $d-2$  vertices of degree 2, a contradiction to  $D(G) = D_1(n, d)$ . Then  $v \in \{x_1, x_2, \dots, x_{d-1}\} \setminus \{x_{i'}\}$ . So the claim is true. Assume  $v = x_{j'}$ , where  $j' \in \{1, 2, \dots, d-1\} \setminus \{i'\}$ . Then  $|j' - i'| \leq 2$ . Without loss of generality, assume  $j' < i'$  (otherwise, we can relabel the vertices of  $P$  as  $x_0, x_1, \dots, x_d$  one by one from the opposite direction). Then  $G \cong G_{n,d,i',j'}$ , where  $1 \leq j' = i' - 1$  or  $i' - 2$ . Thus  $G \in \mathcal{G}_{n,d}$ .  $\square$

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